

Chapter 12

SPLIT AND FACTORED FORMS

12.1 The Concept

Factored forms of numerical operators are used extensively in constructing and applying numerical methods to problems in fluid mechanics. They are the basis for a wide variety of methods variously known by the labels “hybrid”, “time split”, and “fractional step”. Factored forms are especially useful for the derivation of practical algorithms that use implicit methods. When we approach numerical analysis in the light of matrix derivative operators, the concept of factoring is quite simple to present and grasp. Let us start with the following observations:

1. Matrices can be split in quite arbitrary ways.
2. Advancing to the next time level always requires some reference to a previous one.
3. Time marching methods are valid only to some order of accuracy in the step size, h .

Now recall the generic ODE’s produced by the semi-discrete approach

$$\frac{d\vec{u}}{dt} = A\vec{u} - \vec{f} \quad (12.1)$$

and consider the above observations. From observation 1 (we split A) :

$$\frac{d\vec{u}}{dt} = [A_1 + A_2]\vec{u} - \vec{f} \quad (12.2)$$

where $A = [A_1 + A_2]$ but A_1 and A_2 are not unique. For the time march let us choose the simple, first-order,¹ explicit Euler method. Then, from observation 2 (new data \vec{u}_{n+1} in terms of old \vec{u}_n):

$$\vec{u}_{n+1} = [I + hA_1 + hA_2]\vec{u}_n - h\vec{f} + O(h^2) \quad (12.3)$$

or its equivalent

$$\vec{u}_{n+1} = [[I + hA_1][I + hA_2] - h^2[A_1A_2]]\vec{u}_n - h\vec{f} + O(h^2)$$

Finally, from observation 3 (we drop higher order terms $-h^2[A_1A_2]\vec{u}_n$):

$$\vec{u}_{n+1} = [I + hA_1][I + hA_2]\vec{u}_n - h\vec{f} + O(h^2) \quad (12.4)$$

Notice that Eqs. 12.3 and 12.4 have the same formal order of accuracy and, in this sense, neither one is to be preferred over the other. However, their numerical stability can be quite different, and techniques to carry out their numerical evaluation can have arithmetic operation counts that vary by orders of magnitude. Both of these considerations are investigated later. Here we seek only to apply to some simple cases the concept of factoring.

12.2 Factoring Physical Representations — Time Splitting

Suppose we have a PDE that represents both the processes of convection and dissipation. The semi-discrete approach to its solution might be put in the form

$$\frac{d\vec{u}}{dt} = A_c\vec{u} + A_d\vec{u} + (bc) \quad (12.5)$$

where A_c and A_d are matrices representing the convection and dissipation terms, respectively; and their sum forms the A matrix we have considered in the previous sections. Choose again the explicit Euler time march so that

$$\vec{u}_{n+1} = [I + hA_d + hA_c]\vec{u}_n + h(bc) + O(h^2) \quad (12.6)$$

Now consider the factored form

$$\begin{aligned} \vec{u}_{n+1} &= [I + hA_d]([I + hA_c]\vec{u}_n + h(bc)) \\ &= \underbrace{[I + hA_d + hA_c]\vec{u}_n + h(bc)}_{\text{Original Unfactored Terms}} + \underbrace{h^2[A_d]([A_c]\vec{u}_n + (bc))}_{\text{Higher Order Terms}} + O(h^2) \end{aligned} \quad (12.7)$$

¹Second-order time-marching methods are considered later.

and we see that Eq. 12.7 and the original unfactored form Eq. 12.6 have identical orders of accuracy in the time approximation. Therefore, on this basis, their selection is arbitrary. In practical applications² equations such as 12.7 are often applied in a predictor-corrector sequence. In this case one could write

$$\begin{aligned}\tilde{u}_{n+1} &= [I + hA_c]\vec{u}_n + h(bc) \\ \vec{u}_{n+1} &= [I + hA_d]\tilde{u}_{n+1}\end{aligned}\tag{12.8}$$

Factoring can also be useful to form split combinations of implicit and explicit techniques. For example, another way to approximate Eq. 12.6 with the same order of accuracy is given by the expression

$$\begin{aligned}\vec{u}_{n+1} &= [I - hA_d]^{-1}([I + hA_c]\vec{u}_n + h(bc)) \\ &= \underbrace{[I + hA_d + hA_c]\vec{u}_n + h(bc)}_{\text{Original Unfactored Terms}} + O(h^2)\end{aligned}\tag{12.9}$$

where in this approximation we have used the fact that

$$[I - hA_d]^{-1} = I + h[A_d] + h^2[A_d]^2 + \dots$$

if $h \cdot \|A_d\| < 1$, where $\|A_d\|$ is some norm of $[A_d]$. This time a predictor-corrector interpretation leads to the sequence

$$\begin{aligned}\tilde{u}_{n+1} &= [I + hA_c]\vec{u}_n + h(bc) \\ [I - hA_d]\vec{u}_{n+1} &= \tilde{u}_{n+1}\end{aligned}\tag{12.10}$$

The convection operator is applied explicitly, as before, but the diffusion operator is now implicit, requiring a tridiagonal solver if the diffusion term is central differenced. Since numerical stiffness is generally much more severe for the diffusion process, this factored form would appear to be superior to that provided by Eq. 12.8. However, the important aspect of stability has yet to be discussed.

We should mention here that Eq. 12.9 can be derived for a different point of view by writing Eq. 12.6 in the form

$$\frac{u_{n+1} - u_n}{h} = [A_c]u_n + [A_d]u_{n+1} + (bc) + O(h^2)$$

Then

$$[I - hA_d]u_{n+1} = [I + hA_c]u_n + h(bc)$$

which is identical to Eq. 12.10.

²We do not suggest that this particular method is suitable for use. We have yet to determine its stability, and a first-order time-march method is usually unsatisfactory.

12.3 Factoring Space Matrix Operators in 2-D

12.3.1 Mesh Indexing Convention

Factoring is widely used in codes designed for the numerical solution of equations governing unsteady two- and three-dimensional flows. Let us study the basic concept of factoring by inspecting its use on the linear 2-D scalar PDE that models diffusion:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \quad (12.11)$$

We begin by reducing this PDE to a coupled set of ODE's by differencing the space derivatives and inspecting the resulting matrix operator.

A clear description of a matrix finite-difference operator in 2- and 3-D requires some reference to a mesh. We choose the 3×4 point mesh³ shown in the Sketch 12.12. In this example M_x , the number of (interior) x points, is 4 and M_y , the number of (interior) y points is 3. The numbers 11, 12, \dots , 43 represent the location in the mesh of the dependent variable bearing that index. Thus u_{32} represents the value of u at $j = 3$ and $k = 2$.

		⊙	⊙	⊙	⊙	
M_y	⊙	13	23	33	43	⊙
k	⊙	12	22	32	42	⊙
1	⊙	11	21	31	41	⊙
		⊙	⊙	⊙	⊙	
		1	j	\dots	M_x	

(12.12)

Mesh indexing in 2-D.

12.3.2 Data Bases and Space Vectors

The dimensioned array in a computer code that allots the storage locations of the dependent variable(s) is referred to as a *data-base*. There are many ways to lay out a data-base. Of these, we consider only two: (1), consecutively along rows that are themselves consecutive from $k = 1$ to M_y , and (2), consecutively along columns that are consecutive from $j = 1$ to M_x . We refer to each row or column group as a *space vector* (they represent data along lines that are continuous in space) and label

³This could also be called a 5×6 point mesh if the boundary points (labeled ⊙ in the sketch) were included, but in these notes we describe the size of a mesh by the number of *interior* points.

their sum with the symbol U . In particular, (1) and (2) above are referred to as x -vectors and y -vectors, respectively. The symbol U by itself is not enough to identify the structure of the data-base and is used only when the structure is immaterial or understood.

To be specific about the structure, we label a data-base composed of x -vectors with $U^{(x)}$, and one composed of y -vectors with $U^{(y)}$. Examples of the order of indexing for these space vectors are given in Eq. 12.16 part a and b.

12.3.3 Data Base Permutations

The two vectors (arrays) are related by a permutation matrix P such that

$$U^{(x)} = P_{xy}U^{(y)} \quad \text{and} \quad U^{(y)} = P_{yx}U^{(x)} \quad (12.13)$$

where

$$P_{yx} = P_{xy}^T = P_{xy}^{-1}$$

Now consider the structure of a matrix finite-difference operator representing 3-point central-differencing schemes for both space derivatives in two dimensions. When the matrix is multiplying a space vector U , the usual (but ambiguous) representation is given by A_{x+y} . In this notation the ODE form of Eq. 12.11 can be written ⁴

$$\frac{dU}{dt} = A_{x+y}U + (bc) \quad (12.14)$$

If it is important to be specific about the data-base structure, we use the notation $A_{x+y}^{(x)}$ or $A_{x+y}^{(y)}$, depending on the data-base chosen for the U it multiplies. Examples are in Eq. 12.16 part a and b. Notice that the matrices are not the same although they represent the same derivative operation. Their structures are similar, however, and they are related by the same permutation matrix that relates $U^{(x)}$ to $U^{(y)}$. Thus

$$A_{x+y}^{(x)} = P_{xy} \cdot A_{x+y}^{(y)} \cdot P_{yx} \quad (12.15)$$

⁴Notice that A_{x+y} and U , which are notations used in the special case of space vectors, are subsets of A and \vec{u} , used in the previous sections.

$$A_{x+y}^{(x)} \cdot U^{(x)} = \left[\begin{array}{ccc|ccc|ccc} \bullet & x & & & o & & & & & 11 \\ x & \bullet & x & & & o & & & & 21 \\ & x & \bullet & x & & & o & & & 31 \\ & & x & \bullet & & & & o & & 41 \\ \hline o & & & & \bullet & x & & & o & 12 \\ & o & & & x & \bullet & x & & & o & 22 \\ & & o & & & x & \bullet & x & & & 32 \\ & & & o & & & x & \bullet & & & o & 42 \\ \hline & & & & & o & & & \bullet & x & & 13 \\ & & & & & & o & & x & \bullet & x & 23 \\ & & & & & & & o & & x & \bullet & 33 \\ & & & & & & & & o & & x & \bullet & 43 \end{array} \right] \cdot$$

a: Elements in 2-dimensional, central-difference, matrix operator, A_{x+y} , for 3×4 mesh shown in Sketch 12.12.

Data base composed of M_y x-vectors stored in $U^{(x)}$.

Entries for $x \rightarrow x$, for $y \rightarrow o$, for both $\rightarrow \bullet$.

$$A_{x+y}^{(y)} \cdot U^{(y)} = \left[\begin{array}{ccc|ccc|ccc} \bullet & o & & & x & & & & & 11 \\ o & \bullet & o & & & x & & & & 12 \\ & o & \bullet & & & & x & & & 13 \\ \hline x & & & & \bullet & o & & & x & & 21 \\ & x & & & o & \bullet & o & & & x & & 22 \\ & & x & & & o & \bullet & & & & x & & 23 \\ \hline & & & & x & & & & \bullet & o & & 31 \\ & & & & & x & & & o & \bullet & o & 32 \\ & & & & & & x & & o & & \bullet & 33 \\ \hline & & & & & & & & x & & \bullet & o & 41 \\ & & & & & & & & & x & & o & \bullet & 42 \\ & & & & & & & & & & x & & o & \bullet & 43 \end{array} \right] \cdot \quad (12.16)$$

b: Elements in 2-dimensional, central-difference, matrix operator, A_{x+y} , for 3×4 mesh shown in Sketch 12.12.

Data base composed of M_x y-vectors stored in $U^{(y)}$.

Entries for $x \rightarrow x$, for $y \rightarrow o$, for both $\rightarrow \bullet$.

12.3.4 Space Splitting and Factoring

We are now prepared to discuss splitting in two dimensions. It should be clear that the matrix $A_{x+y}^{(x)}$ can be split into two matrices such that

$$A_{x+y}^{(x)} = A_x^{(x)} + A_y^{(x)} \quad (12.17)$$

where $A_x^{(x)}$ and $A_y^{(x)}$ are shown in Eq. 12.22. Similarly

$$A_{x+y}^{(y)} = A_x^{(y)} + A_y^{(y)} \quad (12.18)$$

where the split matrices are shown in Eq. 12.22.

The permutation relation also holds for the split matrices so

$$A_y^{(x)} = P_{xy} A_y^{(y)} P_{yx}$$

and

$$A_x^{(x)} = P_{xy} A_x^{(y)} P_{yx}$$

The splittings in Eqs. 12.17 and 12.18 can be combined with factoring in the manner described in Section 12.2. As an example (first-order in time), applying the implicit Euler method to Eq. 12.14 gives

$$U_{n+1}^{(x)} = U_n^{(x)} + h[A_x^{(x)} + A_y^{(x)}]U_{n+1}^{(x)} + h(bc)$$

or

$$[I - hA_x^{(x)} - hA_y^{(x)}]U_{n+1}^{(x)} = U_n^{(x)} + h(bc) + O(h^2) \quad (12.19)$$

As in Section 12.2, we retain the same first order accuracy with the alternative

$$[I - hA_x^{(x)}][I - hA_y^{(x)}]U_{n+1}^{(x)} = U_n^{(x)} + h(bc) + O(h^2) \quad (12.20)$$

Write this in predictor-corrector form and permute the data base of the second row. There results

$$\begin{aligned} [I - hA_x^{(x)}]\tilde{U}^{(x)} &= U_n^{(x)} + h(bc) \\ [I - hA_y^{(y)}]U_{n+1}^{(y)} &= \tilde{U}^{(y)} \end{aligned} \quad (12.21)$$

$$\begin{aligned}
A_x^{(x)} \cdot U^{(x)} &= \left[\begin{array}{ccc|ccc|ccc} x & x & & & & & & & \\ x & x & x & & & & & & \\ & x & x & x & & & & & \\ & & x & x & & & & & \end{array} \right] \cdot U^{(x)} \\
&\quad \left[\begin{array}{ccc|ccc|ccc} & & & x & x & & & & \\ & & & x & x & x & & & \\ & & & & x & x & x & & \\ & & & & & x & x & & \end{array} \right] \cdot U^{(x)} \\
&\quad \left[\begin{array}{ccc|ccc|ccc} & & & & & & x & x & \\ & & & & & & x & x & x \\ & & & & & & & x & x & x \\ & & & & & & & & x & x \end{array} \right] \\
A_y^{(x)} \cdot U^{(x)} &= \left[\begin{array}{ccc|ccc|ccc} o & & & o & & & & & \\ & o & & & o & & & & \\ & & o & & & o & & & \\ & & & o & & & o & & \end{array} \right] \cdot U^{(x)} \\
&\quad \left[\begin{array}{ccc|ccc|ccc} o & & & o & & & o & & \\ & o & & & o & & & o & \\ & & o & & & o & & & o \\ & & & o & & & & o & \end{array} \right] \cdot U^{(x)} \\
&\quad \left[\begin{array}{ccc|ccc|ccc} & & & o & & & o & & \\ & & & & o & & & o & \\ & & & & & o & & & o \\ & & & & & & o & & \end{array} \right]
\end{aligned} \tag{12.22}$$

The splitting of $A_{x+y}^{(x)}$.

$$\begin{aligned}
A_x^{(y)} \cdot U^{(y)} &= \left[\begin{array}{ccc|ccc|c} x & & & x & & & \\ & x & & & x & & \\ & & x & & & x & \\ \hline x & & & x & & x & \\ & x & & & x & & \\ & & x & & & x & \\ \hline & & & x & & & x \\ & & & & x & & \\ & & & & & x & \\ \hline & & & & x & & x \\ & & & & & x & \\ & & & & & & x \end{array} \right] \cdot U^{(y)} \\
A_y^{(y)} \cdot U^{(y)} &= \left[\begin{array}{ccc|ccc|c} o & o & & & & & \\ o & o & o & & & & \\ & o & o & & & & \\ \hline & & & o & o & & \\ & & & o & o & o & \\ & & & & o & o & \\ \hline & & & & o & o & \\ & & & & o & o & o \\ & & & & & o & o \\ \hline & & & & & & o & o \\ & & & & & & o & o & o \\ & & & & & & & o & o \end{array} \right] \cdot U^{(y)}
\end{aligned} \tag{12.23}$$

The splitting of $A_{x+y}^{(y)}$.

12.4 Second-Order, Implicit, Split & Factored Methods

One can construct $O(h^2)$ methods by using certain second-order time-march methods. For example, apply the trapezoidal method to Eq. 12.14 where the derivative operators have been split as in Eq. 12.17 or 12.18. Let the data base be immaterial and the (bc) be time invariant. There results

$$\left[I - \frac{1}{2}hA_x - \frac{1}{2}hA_y\right]U_{n+1} = \left[I + \frac{1}{2}hA_x + \frac{1}{2}hA_y\right]U_n + h(bc) + O(h^3) \quad (12.24)$$

Factor both sides giving

$$\begin{aligned} & \left[\left[I - \frac{1}{2}hA_x \right] \left[I - \frac{1}{2}hA_y \right] - \frac{1}{4}h^2A_xA_y \right] U_{n+1} \\ &= \left[\left[I + \frac{1}{2}hA_x \right] \left[I + \frac{1}{2}hA_y \right] - \frac{1}{4}h^2A_xA_y \right] U_n + h(bc) + O(h^3) \end{aligned} \quad (12.25)$$

Then notice that the combination $\frac{1}{4}h^2[A_xA_y](U_{n+1} - U_n)$ is proportional to h^3 since the leading term in the expansion of $(U_{n+1} - U_n)$ is proportional to h . Therefore, we can write

$$\left[I - \frac{1}{2}hA_x \right] \left[I - \frac{1}{2}hA_y \right] U_{n+1} = \left[I + \frac{1}{2}hA_x \right] \left[I + \frac{1}{2}hA_y \right] U_n + h(bc) + O(h^3) \quad (12.26)$$

and both the factored and unfactored form of the trapezoidal method are second-order accurate in the time march.

An alternative form of this kind of factorization is the classical ADI (alternating direction implicit) method⁵ usually written

$$\begin{aligned} \left[I - \frac{1}{2}hA_x \right] \tilde{U} &= \left[I + \frac{1}{2}hA_y \right] U_n + \frac{1}{2}hF_n \\ \left[I - \frac{1}{2}hA_y \right] U_{n+1} &= \left[I + \frac{1}{2}hA_x \right] \tilde{U} + \frac{1}{2}hF_{n+1} + O(h^3) \end{aligned} \quad (12.27)$$

For idealized commuting systems the methods given by Eqs. 12.26 and 12.27 differ only in their evaluation of a time-dependent forcing term.

12.5 Importance of Factored Forms in 2 and 3 Dimensions

When the time-march equations are stiff and implicit methods are required to permit reasonably large time steps, the use of factored forms becomes a very valuable tool

⁵A form of the Douglas or Peaceman-Rachfort methods.

for realistic problems. Consider, for example, the problem of computing the time advance in the unfactored form of the trapezoidal method given by Eq. 12.24

$$\left[I - \frac{1}{2}hA_{x+y}\right]U_{n+1} = \left[I + \frac{1}{2}hA_{x+y}\right]U_n + h(bc)$$

Forming the right hand side poses no problem, but finding U_{n+1} requires the solution of a sparse, but very large, set of coupled simultaneous equations having the matrix form shown in Eq. 12.16 part a and b. Furthermore, in real cases involving the Euler or Navier-Stokes equations, each symbol (o, x, \bullet) represents a 4×4 block matrix with entries that depend on the pressure, density and velocity field. Suppose we were to solve the equations directly. The forward sweep of a simple Gaussian elimination fills⁶ all of the 4×4 blocks between the main and outermost diagonal⁷ (e.g. between \bullet and o in Eq. 12.16 part b.). This must be stored in computer memory to be used to find the final solution in the backward sweep. If N_e represents the order of the small block matrix (4 in the 2-D Euler case), the approximate memory requirement is

$$(N_e \times M_y) \cdot (N_e \times M_y) \cdot M_x$$

floating point words. Here it is assumed that $M_y < M_x$. If $M_y > M_x$, M_y and M_x would be interchanged. A moderate mesh of 60×200 points would require over 11 million words to find the solution. Actually current computer power is able to cope rather easily with storage requirements of this order of magnitude. Since they will also have computing speeds of over one gigaflop⁸ direct solvers may then become useful for finding steady-state solutions of practical problems in two dimension. However, a three-dimensional solver would require a memory of approximately

$$N_e^2 \cdot M_y^2 \cdot M_z^2 \cdot M_x$$

words and, for well resolved flow fields, this probably exceeds memory availability for some time to come.

On the other hand, consider computing a solution using the *factored* implicit equation 12.25. Again computing the right hand side poses no problem. Accumulate the result of such a computation in the array (RHS). One can then write the remaining terms in the two-step predictor-corrector form

$$\begin{aligned} \left[I - \frac{1}{2}hA_x^{(x)}\right]\tilde{U}^{(x)} &= (RHS)^{(x)} \\ \left[I - \frac{1}{2}hA_y^{(y)}\right]U_{n+1}^{(y)} &= \tilde{U}^{(y)} \quad O(h^2) \end{aligned}$$

⁶For matrices as small as those shown there are many gaps in this “fill”, but for meshes of practical size the fill is mostly dense.

⁷The lower band is also computed but does not have to be saved unless the solution is to be repeated for another vector.

⁸One billion floating-point operations per second.

which has the same appearance as Eq. 12.21 but is second-order time accurate. The first step would be solved using M_y uncoupled block tridiagonal solvers⁹. Inspecting the top of Eq. 12.22, we see that this is equivalent to solving M_y *one-dimensional* problems, each with M_x blocks of order N_e . The temporary solution $\tilde{U}^{(x)}$ would then be permuted to $\tilde{U}^{(y)}$ and an inspection of the bottom of Eq. 12.23 shows that the final step consists of solving M_x *one-dimensional* implicit problems each with dimension M_y .

12.6 The Delta Form

Clearly many ways can be devised to split the matrices and generate factored forms. One way that is especially useful, for ensuring a correct steady-state solution in a converged time-march, is referred to as the “delta form” and we develop it next.

Consider the unfactored form of the trapezoidal method given by Eq. 12.24, and let the (bc) be time invariant:

$$\left[I - \frac{1}{2}hA_x - \frac{1}{2}hA_y\right]U_{n+1} = \left[I + \frac{1}{2}hA_x + \frac{1}{2}hA_y\right]U_n + h(bc) + O(h^3)$$

From both sides subtract

$$\left[I - \frac{1}{2}hA_x - \frac{1}{2}hA_y\right]U_n$$

leaving the equality unchanged. Then, using the standard definition of the difference operator Δ ,

$$\Delta U_n = U_{n+1} - U_n$$

one finds

$$\left[I - \frac{1}{2}hA_x - \frac{1}{2}hA_y\right]\Delta U_n = h[A_{x+y}U_n + (bc)] + O(h^3) \quad (12.28)$$

Notice that the right side of this equation is the product of h and a term that is identical to the right side of Eq. 12.14, our original ODE. Thus, if Eq. 12.28 converges, it is guaranteed to converge to the correct steady-state solution of the ODE. Now we can factor Eq. 12.28 and maintain $O(h^2)$ accuracy. We arrive at the expression

$$\left[I - \frac{1}{2}hA_x\right]\left[I - \frac{1}{2}hA_y\right]\Delta U_n = h[A_{x+y}U_n + (bc)] + O(h^3) \quad (12.29)$$

This is the delta form of a factored, 2nd-order, 2-D equation.

⁹A block tridiagonal solver is similar to a scalar solver except that small block matrix operations replace the scalar ones, and matrix multiplications do not commute.

The point at which the factoring is made may not effect the order of time-accuracy, but it can have a profound effect on the stability and convergence properties of a method. For example, the unfactored form of a first-order method derived from the implicit Euler time march is given by Eq. 12.19, and if it is immediately factored, the factored form is presented in Eq. 12.20. On the other hand, the *delta form* of the unfactored Eq. 12.19 is

$$[I - hA_x - hA_y]\Delta U_n = h[A_{x+y}U_n + (bc)] \quad O(h)$$

and *its* factored form becomes¹⁰

$$[I - hA_x][I - hA_y]\Delta U_n = h[A_{x+y}U_n + (bc)] \quad O(h) \quad (12.30)$$

In spite of the similarities in derivation, the time convergence properties of Eq. 12.20 and Eq. 12.30 are vastly different.

12.7 Factored Forms Employing Flux Splitting

We shall now investigate factoring in three-dimensions and the use of flux splitting as a means to further split and factor our systems. The three-dimensional system which we will be used here is

$$\frac{dQ}{dt} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = 0 \quad (12.31)$$

with Jacobian matrices $E = AQ$, $F = BQ$, and $G = CQ$ defined in the usual way. Applying implicit Euler time differencing, recasting in “delta” form we have

$$[I + h\delta_x A^n + h\delta_y B^n + h\delta_z C^n] \Delta Q^n = -h(\delta_x E^n + \delta_y F^n + \delta_z G^n) \quad (12.32)$$

Factoring

$$[I + h\delta_x A^n][I + h\delta_y B^n][I + h\delta_z C^n] \Delta Q^n = -h[\delta_x E^n + \delta_y F^n + \delta_z G^n] \quad (12.33)$$

which results (for central space difference approximating δ_x, δ_y , and δ_z) in the block tridiagonal system solution process.

Defining flux-vector splitting in 3D,

$$\begin{aligned} E &= AQ = (A^+ + A^-)Q = E^+ + E^- \\ F &= BQ = (B^+ + B^-)Q = F^+ + F^- \\ G &= CQ = (C^+ + C^-)Q = G^+ + G^- \end{aligned} \quad (12.34)$$

¹⁰Notice that the only difference between the $O(h^2)$ method given by Eq. 12.29 and the $O(h)$ method given by Eq. 12.30 is the appearance of the factor $\frac{1}{2}$ on the left side of the $O(h^2)$ method.

Applying the splitting to Eq. 12.32, we have

$$\begin{aligned} \left[I + h(\delta_x^b A^+ + \delta_x^f A^- + \delta_y^b B^+ + \delta_y^f B^- + \delta_z^b C^+ + \delta_z^f C^-) \right] \Delta Q^n &= \\ -h \left(\delta_x^b E^+ + \delta_x^f E^- + \delta_y^b F^+ + \delta_y^f F^- + \delta_z^b G^+ + \delta_z^f G^- \right) &= R^n \end{aligned} \quad (12.35)$$

with the usual forward and backward difference definitions of δ_x^f, δ_x^b , etc.

The full unfactored algorithm of Eq. 12.35 is not really much different in terms of the operator form than the central difference scheme of Eq. 12.32. Except for the details of the elements in the large banded system and the inherent dissipation of the Flux Split scheme, the unfactored scheme, Eq. 12.35 is still a large block banded system which is difficult and costly to solve. We can reduce the system by factoring as we did before. One possibility is a three-factor scheme

$$\left[I + h\delta_x^b A^+ + \delta_x^f A^- \right] \left[I + \delta_y^b B^+ + \delta_y^f B^- \right] \left[I + \delta_z^b C^+ + \delta_z^f C^- \right] \Delta Q^n = R^n \quad (12.36)$$

which requires three block tridiagonal inversions, and is equivalent to a central differencing and added artificial dissipation algorithm. This is very similar to the algorithm defined in Eq. 12.33. We shall see in the scalar analysis given in Chapter 13 that, the three factor approximate factorization algorithm (for the scalar wave equation using central differencing, periodic analysis and without dissipation) is unconditionally unstable. Now dissipation will mitigate some of the negative aspects of that result and we find at best conditional stability. Again, all the problems come from the three factor form. As an alternative, a two factor scheme can be employed where all the positive terms and all the negative terms are lumped together,

$$\left[I + h(\delta_x^b A^+ + \delta_y^b B^+ + \delta_z^b C^+) \right] \left[I + h(\delta_x^f A^- + \delta_y^f B^- + \delta_z^f C^-) \right] \Delta Q^n = R^n \quad (12.37)$$

This two factor scheme produces a purely upper and lower triangular matrix system (this is obvious from the purely backward and then forward form of the two implicit operators) and can be solved as lower/upper sweeps. The disadvantage of the two factor scheme is that it is harder to vectorize/parallelized, the recursive nature of the sweeps making the identification of a vectorizable/parallelable direction difficult. In contrast, for the three factor scheme, each operator is one-dimensional and can be vectorized/parallelized over one or both of the other directions.

The three-factor implicit central difference scheme suffers from a bad reputation resulting from the linear instability as shown above. In general, for practical problems this doesn't seem to be a real restriction. Nevertheless, one would like to employ schemes which are at least stable in the linear sense. In that regard, an alternative algorithm can be used where flux splitting is employed in one coordinate direction and central differences in the other 2 directions. This produces a two factor implicit

scheme which has central difference characteristics in two coordinate directions (usually the near normal and some other cross flow direction) and an upwind nature in one direction (usually chosen in the major flow direction). The advantages of this scheme is the two factor operator which can be shown to be unconditionally stable in the linear constant coefficient case and the upwind nature of one of the operators which is usually chosen in the direction perpendicular to a shock or flow discontinuity. Consider, for example, a blunt cone at angle of attack. The two factor scheme would use flux splitting in the axial direction, and central differences in the circumferential and body normal directions. Note that in inviscid supersonic axial flow, the scheme could reduce to pure supersonic marching, which can be very efficient.

For demonstration, we flux split the x direction,

$$\frac{dQ}{dt} + \delta_x^b E^+ + \delta_x^f E^- + \delta_y F + \delta_z G = 0$$

where first or second order differences can be employed for δ_x^b and δ_x^f and second order central differences for δ_y and δ_z . The “delta” form of Euler implicit time differencing is given as

$$\begin{aligned} \left[I + h\delta_x^b A^+ + h\delta_y B \right] & \quad \left[I + h\delta_x^f A^- + h\delta_z C \right] \Delta Q^n = \\ -h & \quad \left(\delta_x^b E^+ + \delta_x^f E^- + \delta_y F + \delta_z G \right) = 0 \end{aligned} \quad (12.38)$$

where the $\delta_x^b A^+$ implicit operator is placed with the y operator and the $\delta_x^f A^-$ operator is placed with the z operator. This produces a two-factor scheme which is lower diagonal in x coupled with block tridiagonal in y for the first operator, which can be solved by sweeping in x within an LU decomposition in y . The z operator is handled similarly except that it is upper block diagonal in x and block tridiagonal in z . This produces an efficient algorithm which does not suffer directly from the three-factor linear instability. The first operator can be vectorized in z while the second is vectorized in y .